10579219.txt

=> d	his
-	(FILE 'HOME' ENTERED AT 18:45:10 ON 27 DEC 2007)
L1 L2 L3	FILE 'REGISTRY' ENTERED AT 18:45:26 ON 27 DEC 2007 STRUCTURE UPLOADED 1 S L1 14 S L1 FULL
L4 L5 L6 L7	FILE 'HCAPLUS, CHEMCATS' ENTERED AT 18:46:10 ON 27 DEC 2007 55 S L3 0 S L4 AND ?GARCINOL DERIVATIVE? 46 S L4 AND ?GARCINOL 2 S L6 AND (ALKOXY OR METHOXY OR ETHOXY OR ISOPROPOXY OR BUTOXY

C:\Program Files\Stnexp\Queries\219.str

chain nodes:

7 9 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 35 36 37 38 39 40 41 42

ring nodes:

1 2 3 4 5 6 8 10 11 12 13 14 32 33 34

chain bonds:

3-42 4-41 6-7 7-8 7-9 10-15 11-17 12-16 13-22 14-40 17-18 18-19 19-20 19-21 22-23 23-24 23-25 24-28 25-26 25-27 28-29 29-30 29-31 33-35 35-36 36-37 37-38 37-39

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 8-10 8-14 10-11 11-12 11-32 12-13 13-14 13-34 32-33 33-34 exact/norm bonds :

3-42 4-41 7-9 10-15 12-16 14-40

exact bonds:

6-7 7-8 8-10 8-14 10-11 11-12 11-17 11-32 12-13 13-14 13-22 13-34 17-18 18-19 19-20 19-21 22-23 23-24 23-25 24-28 25-26 25-27 28-29 29-30 29-31 32-33 33-34 33-35 35-36 36-37 37-38 37-39

normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems: containing 1: 8:

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:Atom 9:CLASS10:Atom 11:Atom 12:Atom 13:Atom

14:Atom 15:CLAS\$16:CLAS\$17:CLAS\$18:CLAS\$19:CLAS\$20:CLAS\$21:CLAS\$22:CLAS\$ 23:CLAS\$24:CLAS\$25:CLAS\$26:CLAS\$27:CLAS\$28:CLAS\$29:CLAS\$30:CLAS\$31:CLAS\$32:Atom 33:Atom 34:Atom 35:CLAS\$36:CLAS\$37:CLAS\$38:CLAS\$39:CLAS\$40:CLAS\$41:CLAS\$42:CLAS\$